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ABSTRACT

This paper is an overview of part of the beam optics code development effort in the Accelerator Technology Division at Los Alamos National Laboratory. The aim of this effort is to improve our capability to design advanced beam optics systems. The work reported is being carried out by a collaboration of permanent staff members, visiting consultants, and student research assistants. The main components of the effort are

- building a new framework of common supporting utilities and software tools to facilitate further development,
- research and development on basic computational techniques in classical mechanics and electrodynamics, and
- evaluation and comparison of existing beam optics codes, and support for their continuing development.

OPTICS CODE DEVELOPMENT

The Need for Code Development

At present, many independent beam optics codes exist, but none have all the desired capabilities. The existing codes are typically large, self-contained, batch-oriented programs that communicate via their own uniquely formatted input and output files. Expertise is necessary to use any of them, and modifications are difficult (often even for the author).

To design and operate advanced magnetic optics systems, we need to progress beyond this situation. We would like to do so by building on what has gone before, adding new capabilities while making maximum use of existing software to develop a portable, modular, expandable library of reusable simulation software suitable for both interactive and batch design processes, as well as model support in control systems.

The objective is to create a software development environment that makes it easy to merge, modify, and extend capabilities, with a common user interface to make expertise reusable. The interface should allow various control

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mechanisms (such as batch, interactive, or automatic) for running the codes and should use standardized optimization, fitting, and graphics utilities. The system must be capable of highly-accurate simulations, with the flexibility to allow trade-offs between speed and accuracy by using various levels of physics approximation. A key prerequisite is the definition of a simple and practical internal representation of a general beamline and of a general description of the beam.

Full implementation of these goals is a large undertaking, but plans can be laid so that small practical steps accumulate in that direction. The following sections describe these plans in more detail, along with implementation steps being taken or considered.

Internal Data Structure

The backbone of the system must be a simple, portable, internal data structure with well-defined units and variables. This probably means standard FORTRAN 77 common blocks, without computer specific extensions, and cannonical MKS particle coordinates as used by MARYLIE, COSY and MAD. The common blocks should contain a general machine description consisting of element sequence arrays, with the ability to repeat (nested) groups of elements, along with a simple, flexible, and efficient indexing scheme for accessing element parameter blocks. The common blocks should also contain a general beam description, allowing at least sets of particle coordinates or beam moments (σ-matrices) at selected locations. A set of database service routines could also be provided to make data access even more flexible and portable.

Beam Descriptions

There are three major possibilities for representing an accelerator beam. Our ideal system should allow all of them and provide means for transforming among them.

- Particle Sets: We need a standard particle set generator code to produce all the commonly used beam distributions in the forms needed by the optics codes. A start has been made, based on the BEAMGEN program from PATH, to collect every known algorithm for generating rays or particle sets. Our interim standard output is a simple ASCII file of the type used by MARYLIE, with one particle per record $(x, p_x, y, p_y, \tau, p_\tau)$. Generic phase-space scatter plot and analysis programs have been written to process this standard particle file.

- Beam Moments: The σ matrices as used by TRANSPORT may be considered second moments of the beam distribution. The higher moments of the distribution need to be considered for more accurate design, and a

standard notation for them needs to be defined. The MARYLIE monomial sequence can be used as an interim standard storage format. Twiss parameters and higher moment invariants are related and can be used as input parameters for the particle set generators.

- Beam Distribution Functions: No standard format has been defined. Maximum entropy techniques may be useful for estimating distribution functions. Sums of Gaussians with adjustable amplitudes are being used to represent beam distributions for space-charge calculations.

Physics Levels

Design can be carried out to various levels of physics approximation, ranging from fast and simple to slow and accurate. The general data structure needs to be flexible enough to support all the commonly used formulations of accelerator physics. That is, while the physics modules themselves may use very different techniques, they should all be able to draw their machine parameters from, and store their results in, the common data structure. The design of this data structure must therefore allow for at least the following variations:

- Ray tracing can be done either by particle mapping or by trajectory integration. Mapping codes can use various map representations (Matrices, Lie Polynomials, or Differential Algebra) expanded to various orders.

- Magnetic fields can be represented by various expansions, nominal formulas, or empirical data tables. Fringe-field effects can also be computed in various approximations ranging from simple correction factors to full numerical integration of trajectories.

- Space-charge effects can also be computed to various levels of accuracy, ranging from simple approximations up to full particle-in-cell code calculations.

Reusing Software.

To get the new system started, we need to make maximum use of existing software. One way to do this is to separate the input file parser from a major operational code and use it to initialize the standard commons. The tracking routines that propagate the beam through the machine would then be modified so that they can be driven by the new standard commons. New routines would then be written to display and modify the contents of the standard commons, at first by simple manual editing. A module would then be written to generate the operational code's input deck from the current contents of the standard common. As other operational codes receive this treatment, the set of programs to map their various input file formats to and from the standard commons will, in itself, constitute a useful translation facility. The

initial operating capability of the new system would then be benchmarked on some familiar test cases. Work could then begin on new modules such as interactive graphic input, output, and control that would serve all the participating operational codes.

Control Mechanisms

It is desirable to have several options for controlling the basic physics routines that propagate a beam representation using the current machine parameters. An interactive system could allow manual adjustment of machine parameters, with prompt updates of diagnostic displays, such as ellipse plots. Prototypes of several such systems are under development [1,2]. A general purpose optimizer could also be used to adjust the machine parameters. Because design is generally aimed at achieving specified beam characteristics, the merit function guiding the optimizer is often calculated from the beam description. A batch process, using the same instructions as the interactive system, should be possible when the slow and accurate physics is being used. Finally, a set of common graphics modules should be able to display the results, no matter how they are obtained.

Optimizer Development

Optimizers and equation solvers are essential design tools. For our purposes, good ones need the following virtues: They should be FORTRAN callable subroutines, leaving the elaborate main physics codes in control. Most available optimizers are written the other way around, calling the function to be minimized as often as they please. They should be extremely frugal with function calls, because these can each be a very expensive model computation, and they should be as robust as possible, using the best available search algorithms to find the solution.

Significant effort has been directed toward the development of such optimizers and solvers. An efficient quasi-linear system solver was written using a multidimensional inverse interpolation algorithm (MDII)[3] and fully integrated into MARYLIE to provide a new parameter fitting capability. Available optimizer techniques and codes were surveyed, and a new optimizer (QMIN) was written addressing the above requirements. QMIN uses quadratic fitting of the Hessian to the best previous points to speed convergence. It performed very well on a suite of standard test problems [4]. Four of the most suitable optimizers (including QMIN) have been installed in a test version of MARYLIE for evaluation on real problems. An early version of QMIN is also operational in the McDonnell Douglas version of TRAVEL [5].

NEW CALCULATIONAL METHODS

This section surveys part of the basic research being done in new computational techniques in classical mechanics and electrodynamics.

Mechanics

A new, explicit, high-order multipoint symplectic Adams integrator for particle tracking has been written and tested for simple nonlinear Hamiltonians [6]. It does not require knowledge of higher derivatives of the forces.

A new technique is under development for generating high-order symplectic maps of machine elements by integrating the Hamiltonian-Jacobi equation using Differential Algebra methods [7,8] .

The use of the moments of the distribution function as dynamical variables is under investigation. This includes the search for new moment invariants that are higher-order generalizations of the emittance [9].

Electrodynamics

The code CHARLIE uses Lie algebraic methods to study the effects of space charge [10]. CHARLIE is based on MARYLIE and, at present, can handle only 2-D space-charge problems with free-space boundary conditions.

A method of representing an arbitrary charge distribution by a superposition of regularly distributed Gaussian particles has been completed to fifth order for 3-D, using free-space boundaries. The corresponding field expansions are computed using Differential Algebra. This method has been tested statically but not yet in a dynamics code. It promises to be efficient and accurate for 3-D problems and can be made to handle 3-D conducting boundaries.

A formalism for computing the vector potential of Lambertson coils is under development [11]. The associated subroutines for use in tracking codes are being written.

WORK ON OPERATIONAL CODES

Improvements in Operational Codes

The operational codes in current use for beam optics design in the Accelerator Technology Division include MARYLIE, GIOS, COSY, MOTER, TRANSOPTR, TRANSPORT, TRACE-3D, and others. Modifications are often necessary in the course of the work. The following modifications have been carried out recently, either by or in collaboration with the authors of the codes.

The capabilities of MARYLIE [12] continue to grow. Recent additions include a general fitting procedure [3], a set of experimental optimization routines, and the ability to track moments. The ability to compute maps for

strings of permanent magnet quadrupoles by numerical integration has also been added.

Some small improvements have been made to the linear space-charge routines in GIOS [13]. The new fifth-order code COSY [14] is now operational and can handle permanent magnet quadrupoles.

MOTER is an optimizing version of RAYTRACE. It was used extensively to design the Argonne Telescope experiment. Recent improvements include the ability to trace sextupole, octupole and decapole magnets.

TRANSOPTR [15,16] can now design beamlines containing dipole and quadrupole rf elements, which can be used for chromatic aberration correction. The transfer matrix formulas for these rf elements were calculated using the computer algebra system SMP, which also generated FORTRAN code for these elements. The computations were done to second order, although the automatic process could readily have generated higher-order elements.

Code Benchmarking

Benchmarking operational codes by comparing them with each other, and with experiments, is necessary to build confidence in the codes. The following benchmarking exercises were carried out recently.

The codes MARYLIE, MOTER, NIREC (numerical trajectory integration), and SYMPOPT (experimental symplectic integration code) were compared on a beam-expansion problem without space charge. Except for SYMPOPT, they agreed to within 0.5 microradian for this benchmark.

For a space-charge benchmark, the problem used was a drift space transporting a space-charge-dominated beam with 3-D free-space boundaries. On this problem, the codes TRACE-3D, TRANSOPTR, TRANSPORT, and PATH (nonlinear) agreed to better than 5%.

The Los Alamos/Argonne telescope was designed with MOTER and checked with MARYLIE and GIOS. The telescope worked [17] and produced measured aberration coefficients in good agreement with the code predictions when the correct fringe-field form was used.

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